Lecture 18: EM

Fall 2022

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The instructor gratefully acknowledges Dan Roth, Vivek Srikuar, Sriram Sankararaman, Fei Sha, Ameet Talwalkar, Eric Eaton, and Jessica Wu whose slides are heavily used, and the many others who made their course material freely available online.

Final Exam

- ❖ Official exam time 12/9 11:30am -- 2:30pm
- Closed-book in-person exam at Moore Hall 100
- We expect to complete the grading in about a week
- The final grade will be computed based on the formulation in Lecture 1

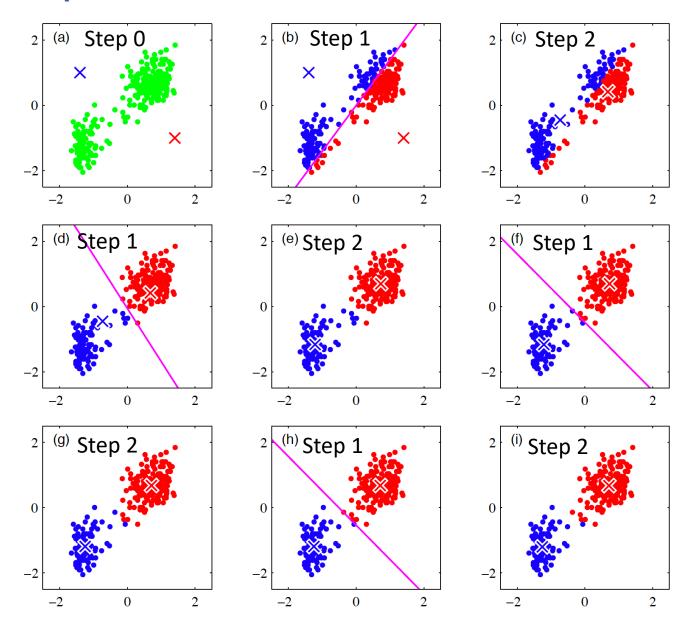
Cover everything until today's lecture

Course evaluation survey

- Please complete the course survey at MyUCLA by 12/2
 - Your feedback is important for us as we continue improving the courses and incorporating new materials
 - 2 bonus points for the final for students filling out the survey
 - Your response is anonymous

Unsupervised Learning

Recap: K-Means



Recap: K-means algorithm

- **Step 0:** randomly assign the cluster centers $\{\mu_k\}$
- **Step 1:** Minimize J over $\{r_{nk}\}$ -- Assign every point to the closest cluster center

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_{j} \|\boldsymbol{x}_n - \boldsymbol{\mu}_j\|_2^2 \\ 0 & \text{otherwise} \end{cases}$$

Step 2: Minimize J over $\{\mu_k\}$ -- update the cluster centers

$$oldsymbol{\mu}_k = rac{\sum_n r_{nk} oldsymbol{x}_n}{\sum_n r_{nk}}$$

Loop until it converges

Recap: K-means algorithm

- **Step 0:** randomly assign the cluster centers $\{\mu_k\}$
- **Step 1:** Minimize J over $\{r_{nk}\}$ -- Assign every point to the closest cluster center

$$r_{nk} = \left\{ egin{array}{ll} 1 & ext{if } k = rg \min_j \|m{x}_n - m{\mu}_j\|_2^2 \\ 0 & ext{otherwise} & ext{Assign data to clusters based on the model (E-step)} \end{array}
ight.$$

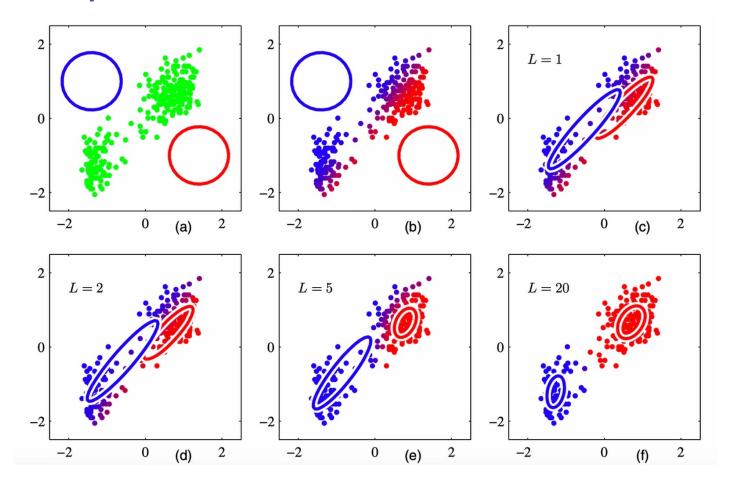
Step 2: Minimize J over $\{\mu_k\}$ -- update the cluster centers

$$oldsymbol{\mu}_k = rac{\sum_n r_{nk} oldsymbol{x}_n}{\sum_n r_{nk}}$$

Updating the model (M-Step)

Loop until it converges

Recap: GMM



Assume each cluster can be modeled by a Gaussian with cluster center μ_k and covariance matrix Σ_k i.e., $P(x|cluster=k) = N(x|\mu_k, \Sigma_k)$ Lec 18: EM / GMM

We will go back to explain formulation later

From K-means to GMM

- Step 0: randomly assign the cluster centers $\{\mu_k\}$ and covariance matrices $\{\Sigma_k\}$
- Step 1: Assign every point to the cluster based on posterior distribution $P(z_n = k | x_n)$

$$p(z_n = k | \boldsymbol{x}_n) = \frac{p(\boldsymbol{x}_n | z_n = k) p(z_n = k)}{p(\boldsymbol{x}_n)} = \frac{p(\boldsymbol{x}_n | z_n = k) p(z_n = k)}{\sum_{k'=1}^{K} p(\boldsymbol{x}_n | z_n = k') p(z_n = k')}$$

Step 2: update the cluster centers $\{\mu_k\}$, and covariance matrices $\{\Sigma_k\}$ based on soft assignment $\gamma_{nk} = P(z_n = k | x_n)$

$$\omega_k = \frac{\sum_n \gamma_{nk}}{\sum_k \sum_n \gamma_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} \boldsymbol{x}_n$$

$$oldsymbol{\Sigma}_k = rac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (oldsymbol{x}_n - oldsymbol{\mu}_k) (oldsymbol{x}_n - oldsymbol{\mu}_k)^{\mathrm{T}}$$

Loop until it converges

 γ_{nk} is similar to r_{nk} in K-means, but $\gamma_{nk} \in (0,1), r_{nk} \in \{0,1\}$

Unsupervised Learning – Expectation Maximization (EM)

Roadmap

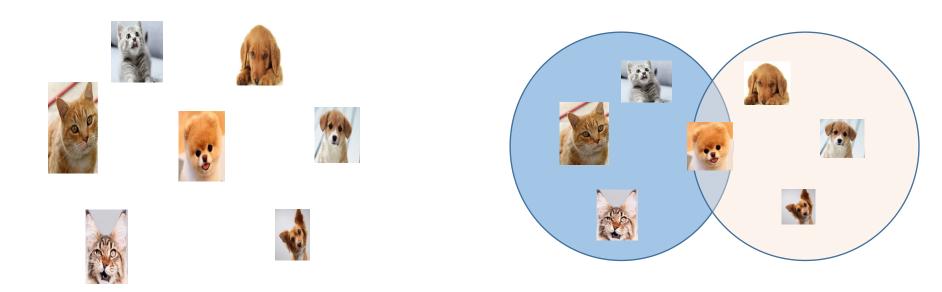
The goal of EM algorithm

A numerical example

GMM (instance of EM)

How about unsupervised learning

 \bullet In unsupervised learning, we only observed input distribution P(X)



MLE in unsupervised learning

- \bullet We only have the observation of P(X)
- We make assumptions to model $P(X, Y \mid \Theta)$
- •• We know $P(X \mid \Theta) = \sum_{Y} P(X, Y \mid \Theta)$
- * Therefore, MLE is $argmax_{\Theta}P(X \mid \Theta)$

$$= \operatorname{argmax}_{\Theta} \sum_{Y} P(X, Y \mid \Theta)$$

$$= \operatorname{argmax}_{\Theta} \log \sum_{Y} P(X, Y \mid \Theta)$$

EM algorithm

- **EM** algorithm essentially solves $\arg\max_{\Theta}\log\sum_{Y}P(X,Y\mid\Theta)$ by iteratively updating Θ (come back to this point later)
 - \clubsuit At iteration t, the model Θ^t
 - \bullet E-Step: Estimate P(Y | X, Θ^t)

 Step 1 in GMM
 - M-Step: Optimize

$$\max_{\Theta} \sum_{\mathbf{Y}} [P(\mathbf{Y} \mid \mathbf{X}, \mathbf{\Theta}^t) \log P(\mathbf{X}, \mathbf{Y} | \mathbf{\Theta})]$$
 Step 2 in GMM

In general, it converges to a local maximum

Roadmap

The goal of EM algorithm

A numerical example

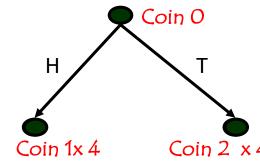
GMM (instance of EM)

Three Coins Example

- We observe a series of coin tosses generated in the following way:
- A person has three coins.
 - Coin 0: probability of Head is α
 - Coin 1: probability of Head p
 - Coin 2: probability of Head q

Consider the following coin-tossing scenarios:

Scenario I



Toss coin 0
If Head – toss coin 1 x 4 times;
o/w – toss coin 2 x 4 times

Observing the sequence HHHHT, THTHT, HHHHT, HHTTH produced by Coin 0, Coin1 and Coin2

Question: Estimate most likely values for α , p, q (the probability of H in each coin) and the probability to use each of the coins

Supervised Learning

Scenario I

★ Toss coin 0

If Head – toss coin 1 x 4 times;

o/w – toss coin 2 x 4 times

Observing the sequence HHHHT, THTHT, HHHHT, HHTTH produced by Coin 0, Coin1 and Coin2

Question: Estimate most likely values for α , p, q (the probability of H in each coin) and the probability to use each of the coins

Coin O

 α =3/4, p=8/12, q=2/4

Scenario II

★ Toss coin 0

Coin 1x 4

Coin 2 x 4

If Head – toss coin 1 x 4 times;

o/w – toss coin 2 x 4 times

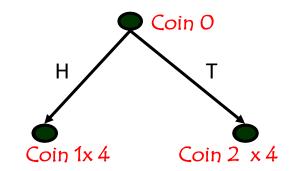
Now we only observe outcomes from coins 1 & 2 ?HHHT, ?HTHT, ?HHHHT, ?HTTH

Coin O

Question: Estimate most likely values for α , p, q (the probability of H in each coin) and the probability to use each of the coins

Guess Coin 0 based on the model

Toss coin 0 If Head – toss coin 1 x 4 times; o/w – toss coin 2 x 4 times



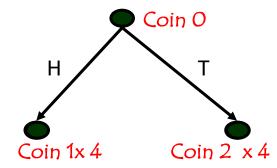
Assume α =3/4, p=2/3, q=1/2 If we observe the outcome sequence is ?HHHT

Question: How likely the sequence is from Coin 1 vs Coin 2

hint: Bayes' theorem

Guess Coin 0 based on the model

Toss coin 0
If Head – toss coin 1 x 4 times;
o/w – toss coin 2 x 4 times



Assume
$$\alpha = 3/4$$
, p=2/3, q=1/2

Question: How likely the sequence ?HHHT is from Coin 1 vs Coin 2

$$P(HHHHT) = \frac{3}{4} \times \left(\frac{2}{3}\right)^{3} \times \left(\frac{1}{3}\right)$$

$$P(THHHT) = \frac{1}{4} \times \left(\frac{1}{2}\right)^{3} \times \left(\frac{1}{2}\right)$$

$$P(coin0 = H|?HHHT) = \frac{P(HHHHT)}{P(HHHHT) + P(THHHT)}$$

Intuition of EM algorithm

- Use an iterative approach for estimating the parameters:
 - Guess the probability that a given data point came from Coin 1 or 2; Generate fictional labels, weighted according to this probability.
 - Then, compute the most likely value of the parameters. [supervised learning]
 - Compute the likelihood of the data given this model.
 - Re-estimate the parameter setting: set them to maximize the likelihood of the data.

Step 1: Random initialization

Guess the probability that a given data point came from Coin 1 or 2 randomly

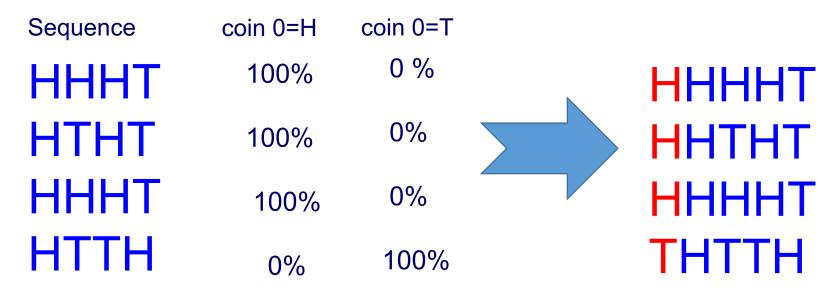
Coin 0: probability of Head is α Coin 1: probability of Head p Coin 2: probability of Head q

Sequence	coin 0=H	coin 0=H coin 0=T	
HHHT	100%	0 %	
HTHT	100%	0%	
HHHT	100%	0%	
HTTH	0%	100%	

Coin 0: probability of Head is α Coin 1: probability of Head p

Coin 2: probability of Head q

Now, compute the most likely value of the parameters. [Supervised Learning]



E-STEP - guess labels

Coin 0: probability of Head is α Coin 1: probability of Head p

Coin 2: probability of Head q

Now, compute the most likely value of the parameters.

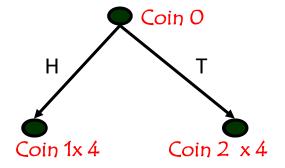
Sequence

$$\alpha_1 = \frac{3}{3+1} = \frac{3}{4}$$

$$p_1 = \frac{8}{8+4} = \frac{2}{3}$$

$$q_1 = \frac{2}{2+2} = \frac{1}{2}$$

 $P(coin \ 0 \mid Sequence; \alpha_1, p_1, q_1)$



Compute the likelihood of the data given this model

 $\alpha_1 p_1^{\#H} (1 - p_1)^{\#T}$

Sequence

HHHT HTHT HHHT HTTH coin 0 =H

$$\frac{3}{4} \left(\frac{2}{3}\right)^{3} \frac{1}{3}$$

$$\frac{3}{4} \left(\frac{2}{3}\right)^{2} \left(\frac{1}{3}\right)^{2}$$

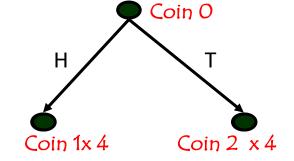
$$\frac{3}{4} \left(\frac{2}{3}\right)^{3} \frac{1}{3}$$

$$\frac{3}{4} \left(\frac{2}{3}\right)^{2} \left(\frac{1}{3}\right)^{2}$$

 $\frac{(1 - \alpha_1)q_1^{\#H}(1 - q_1)^{\#T}}{\text{coin } 0 = T} \qquad \alpha_1 = \frac{3}{4}$

$$\frac{\frac{1}{4}\left(\frac{1}{2}\right)^{3} \frac{1}{2}}{\frac{1}{4}\left(\frac{1}{2}\right)^{2} \left(\frac{1}{2}\right)^{2}} \qquad p_{1} = \frac{2}{3}$$

$$\frac{\frac{1}{4}\left(\frac{1}{2}\right)^{3} \frac{1}{2}}{\frac{1}{4}\left(\frac{1}{2}\right)^{2} \left(\frac{1}{2}\right)^{2}} \qquad q_{1} = \frac{1}{3}$$



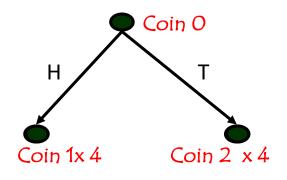
$$P(coin 0 = H \mid Seq) = \frac{P(coin0 = H, Seq)}{P(coin0 = H, Seq) + P(coin0 = T, Seq)}$$

Compute P(coin0, Seq)

Sequence
$$\alpha_1 p_1^{\#H} (1-p_1)^{\#T}$$
 $coin 0=H$ $coin 0=T$ $coin$

$$\frac{0.074}{0.074 + 0.0156} = 82.6\%$$

$$P(coin 0 = H \mid Seq) = \frac{P(coin0 = H, Seq)}{P(coin0 = H, Seq) + P(coin0 = T, Seq)}$$



 \bullet Compute $P(coin \ 0 = H \mid Seq)$

нннт
HTHT
HHHT
HTTH

$$\alpha_1 = \frac{3}{4}$$

$$p_1 = \frac{2}{3}$$

$$q_1 = \frac{1}{3}$$

$$\frac{0.074}{0.074 + 0.0156} = 82.6\%$$

Step 2: Maximum Conditional Likelihood

Coin 0: probability of Head is α Coin 1: probability of Head p Coin 2: probability of Head q

C - ft | - | - | - - - : - - - - - + /

Now, compute the most likely value of the parameters. [recall the scenario I]

	coin 0=H	coin 0=T		Soft label assignment/ weighted instance		
HHHT HTHT	82.6% 70.3%	17.4% - 29.7% -	0.174	HHHHT THHHT HHTHT		
HHHT	82.6% 70.3%	17.4% 29.7%	0.297 0.826	THTHT HHHHT		
			0.703	THHHT HHTTH THTTH		

Step 2: Maximum Conditional Likelihood

Coin 0: probability of Head is α Coin 1: probability of Head p Coin 2: probability of Head q

Now, compute the most likely value of the parameters. [recall the scenario I]

$$\begin{array}{ll} 0.826 & \text{HHHHT} \\ 0.174 & \text{THHHT} \\ 0.703 & \text{HHTHT} \\ 0.297 & \text{THTHT} \\ 0.826 & \text{HHHHT} \\ 0.174 & \text{THHHT} \\ 0.703 & \text{HHTTH} \\ \end{array} \qquad \begin{array}{ll} \alpha_2 = \frac{0.826 \times 2 + 0.703 \times 2}{4} = 0.765 \\ \hline 0.826 \times 6 + 0.703 \times 4 \\ \hline 0.826 \times 8 + 0.703 \times 8 \\ \hline 0.826 \times 8 + 0.703 \times 8 \\ \hline 0.174 \times 6 + 0.297 \times 4 \\ \hline 0.174 \times 8 + 0.297 \times 8 \\ \hline 0.297 & \text{THTTH} \end{array} \qquad \begin{array}{ll} \alpha_2 = \frac{0.826 \times 2 + 0.703 \times 2}{4} = 0.635 \\ \hline 0.826 \times 8 + 0.703 \times 8 \\ \hline 0.174 \times 6 + 0.297 \times 4 \\ \hline 0.174 \times 8 + 0.297 \times 8 \\ \hline \end{array} = 0.592$$

$$P(coin 0 = H \mid Seq) = \frac{P(coin0 = H, Seq)}{P(coin0 = H, Seq) + P(coin0 = T, Seq)}$$

Compute P(coin0 | Seq)

$$\alpha_2 = 0.765$$

$$p_2 = 0.635$$

$$q_2 = 0.592$$

HTTH

Sequence

Intuition of EM algorithm

- Use an iterative approach for estimating the parameters:
 - Guess the probability that a given data point came from Coin 1 or 2; Generate fictional labels, weighted according to this probability.
 - Then, compute the most likely value of the parameters. [supervised learning]
 - Compute the likelihood of the data given this model.
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EM algorithm

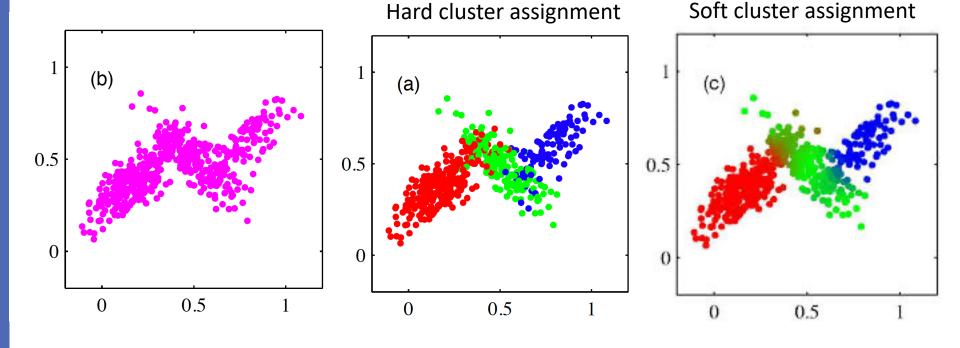
- **EM** algorithm essentially solves $\arg\max_{\Theta}\log\sum_{Y}P(X,Y\mid\Theta)$ by iteratively updating Θ (come back to this point later)
 - \clubsuit At iteration t, the model Θ^t
 - \bullet E-Step: Estimate P(Y | X, Θ^t)
 - M-Step: Optimize $\max_{\Omega} \sum_{Y} [P(Y \mid X, \Theta^{t}) \log P(X, Y \mid \Theta)]$
- In general, it converges to a local maximum

Gaussian Mixture Models

Recap: Gaussian mixture models

Assume the probability density function for x as

$$p(oldsymbol{x}) = \sum_{k=1}^K \omega_k N(oldsymbol{x} | oldsymbol{\mu}_k, oldsymbol{\Sigma}_k)$$



Iterative procedure (similar to k-means)

Let θ represent all parameters $\{\omega_k, \mu_k, \Sigma_k\}$

Step 0: initialize θ with some values (random or otherwise)

Step 1: compute γ_{nk} using the current $\boldsymbol{\theta}$

Step 2: update $oldsymbol{ heta}$ using the just computed γ_{nk}

Step 3: go back to Step 1

E-step: Estimate γ_{nk}

- $ightharpoonup \gamma_{nk} = P(z_n = k | x_n)$ e.g., probability x_n belongs to the red cluster, given the input and model the assignment of z_n to cluster k
- posterior probability

$$p(z_n = k | \boldsymbol{x}_n) = \frac{p(\boldsymbol{x}_n | z_n = k) p(z_n = k)}{p(\boldsymbol{x}_n)} = \frac{p(\boldsymbol{x}_n | z_n = k) p(z_n = k)}{\sum_{k'=1}^{K} p(\boldsymbol{x}_n | z_n = k') p(z_n = k')}$$

M-Step:Parameter estimation for GMMs

- \clubsuit If cluster assignments are observed $\{z_n\}$ are given
 - We know the cluster of each point
 - ❖ Let $\gamma_{nk} \in [0, 1]$ is a soft assignment of instance n to cluster k,
- Then the maximum likelihood estimation is

$$\omega_k = \frac{\sum_n \gamma_{nk}}{\sum_k \sum_n \gamma_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} \boldsymbol{x}_n$$
$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k) (\boldsymbol{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

$$\omega_k = \frac{\sum_n \gamma_{nk}}{\sum_k \sum_n \gamma_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} \boldsymbol{x}_n$$
$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k) (\boldsymbol{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

- For ω_k : count the number of data points whose z_n is k and divide by the total number of data points (note that $\sum_k \sum_n \gamma_{nk} = N$)
- For μ_k : get all the data points whose z_n is k, compute their mean
- For Σ_k : get all the data points whose z_n is k, compute their covariance matrix

GMM algorithm

- **Step 0:** randomly assign the cluster centers $\{\mu_k\}$ and covariance matrices $\{\Sigma_k\}$
- Step 1: Assign every point to the cluster based on posterior distribution $P(z_n = k | x_n)$

$$p(z_n = k | \boldsymbol{x}_n) = \frac{p(\boldsymbol{x}_n | z_n = k) p(z_n = k)}{p(\boldsymbol{x}_n)} = \frac{p(\boldsymbol{x}_n | z_n = k) p(z_n = k)}{\sum_{k'=1}^{K} p(\boldsymbol{x}_n | z_n = k') p(z_n = k')}$$

Step 2: update the cluster centers $\{\mu_k\}$, and covariance matrices $\{\Sigma_k\}$ based on soft assignment $\gamma_{nk} = P(z_n = k | x_n)$

$$egin{aligned} \omega_k &= rac{\sum_n \gamma_{nk}}{\sum_k \sum_n \gamma_{nk}}, \quad oldsymbol{\mu}_k &= rac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} oldsymbol{x}_n \ oldsymbol{\Sigma}_k &= rac{1}{\sum_n \gamma_{nk}} \sum_n \gamma_{nk} (oldsymbol{x}_n - oldsymbol{\mu}_k) (oldsymbol{x}_n - oldsymbol{\mu}_k)^{\mathrm{T}} \end{aligned}$$

Loop until it converges

 γ_{nk} is similar to r_{nk} in K-means, but $\gamma_{nk} \in (0,1), r_{nk} \in \{0,1\}$

Generative v.s Discriminative Models

Example







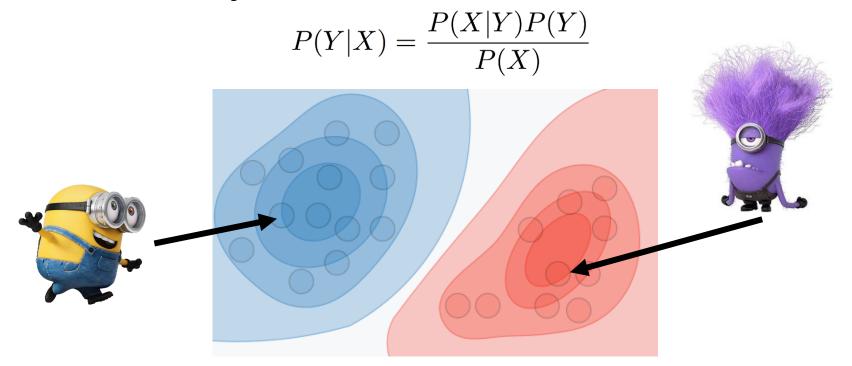






Generative (e.g., Naïve Bayes)

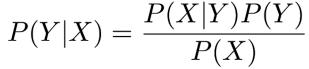
- \Leftrightarrow Estimate P(Y|X) through P(X,Y)
- MLE: $\max_{\theta} \sum_{i=1..n} \log P(y_i, x_i)$

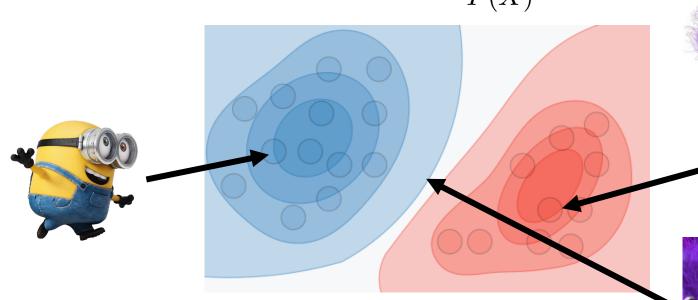


What is the input instances X look like if they belongs to the class Y

Generative (e.g., Naïve Bayes)

- \Leftrightarrow Estimate P(Y|X) through P(X,Y)
- MLE: $\max_{\theta} \sum_{i=1..n} \log P(y_i, x_i)$

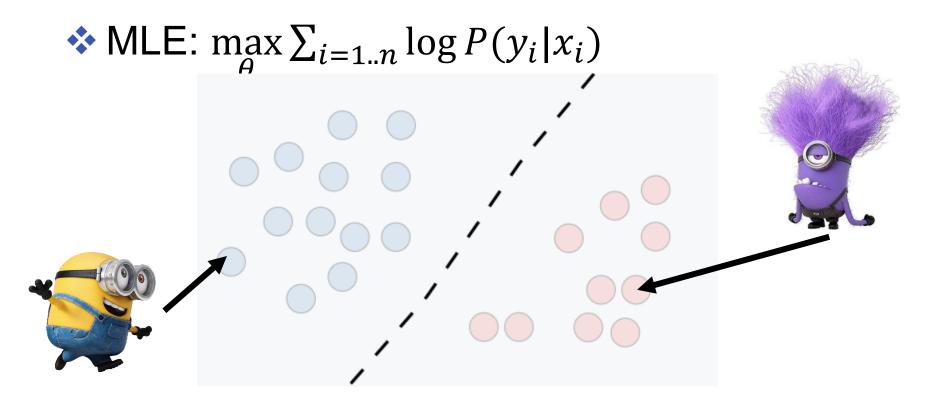




What is the input instances X look like if they belongs to the

Discriminative (e.g., logistic regression, SVM)

 \Leftrightarrow Estimate P(Y|X)

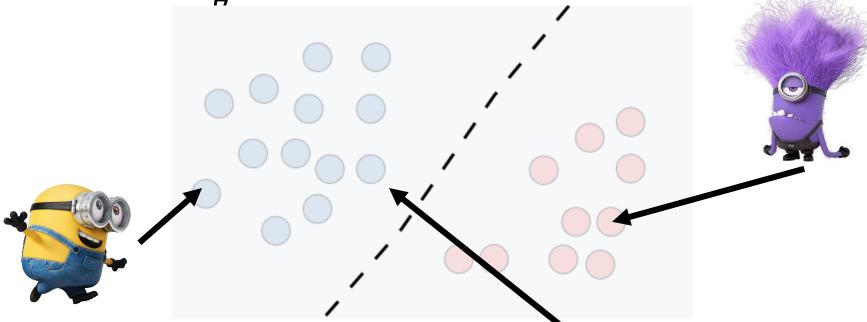


What features can be used to differentiate between different classes

Discriminative (e.g., logistic regression, SVM)

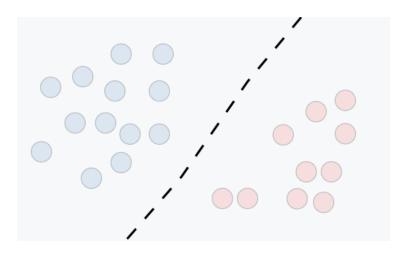
 \Leftrightarrow Estimate P(Y|X)

 \bullet MLE: $\max_{\theta} \sum_{i=1..n} \log P(y_i|x_i)$



What features can be used to differentiate between different cla

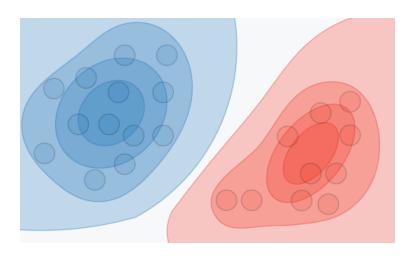
Discriminative vs Generative Models



Estimate P(Y|X)

MLE: $\max_{\theta} \sum_{i=1..n} \log P(y_i|x_i)$

Discriminative



Estimate P(Y|X) through P(X,Y)MLE: $\max_{\theta} \sum_{i=1..n} \log P(y_i, x_i)$

Generative

What features can be used to differentiate between different classes

A retrospective look at the course

Learning = generalization

"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E."

Tom Mitchell (1999)

We saw different "models"

what kind of a function should a learner learn

- ***** K-NN
- Linear classifiers

Decision trees

Non-linear classifiers, feature transformations, neural networks

Different learning protocols

Supervised learning

- A teacher supplies a collection of examples with labels
- The learner has to learn to label new examples using this data

Unsupervised learning

No teacher, learner has only unlabeled examples

The theory of machine learning

Mathematically defining learning

- Entropy (information theorem)
- Probably Approximately Correct (PAC) Learning
- ❖ MLE, MAP
- SGD (optimization)

Some general recipes in ML

- Empirical Loss Minimization
 - Define loss and regularizer -> SGD
- Deep Learning
 - Define model architecture -> SGD
- Probabilistic models
 - \bullet Define model P(Y|X) or P(X,Y)
 - -> MLE, MAP -> SGD, or closed form

Next Step

- If you're interested in ML/AI here are some relevant courses
 - CS145, CS148 have significant overlap w/ CM146 but focus more on data.
 - CS161 (AI) some overlap w/ cM146, but focuses on logic, reasoning, search
 - CS188 (NLP) ML applications in NLP
 - Graduate-level courses deep learning, NLP, Computer vision, probabilistic reasoning, etc...

Practical advices

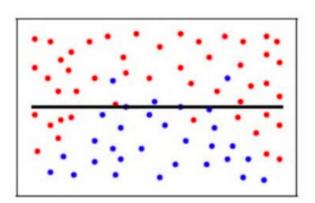
Bias and variance

Every learning algorithm requires assumptions about the hypothesis space.

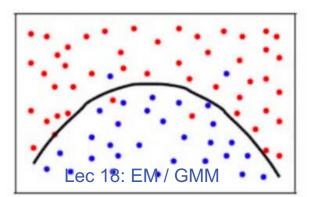
Eg: "My hypothesis space is

- …linear"
- ...decision trees with 5 nodes"
- ...deep neural network with 12 layers"

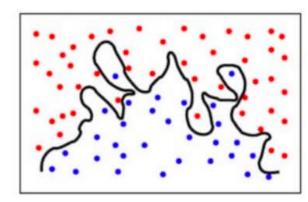
Underfitting







Overfitting



Managing bias and variance

- Decision trees of a fixed depth
 - Increasing depth decreases bias, increases variance
- SVMs
 - Stronger regularization (i.e., smaller C in our formulation) increases bias, decreases variance
- K nearest neighbors
 - Increasing k generally increases bias, reduces variance
- Other approaches: Drop out, Ensemble, etc...

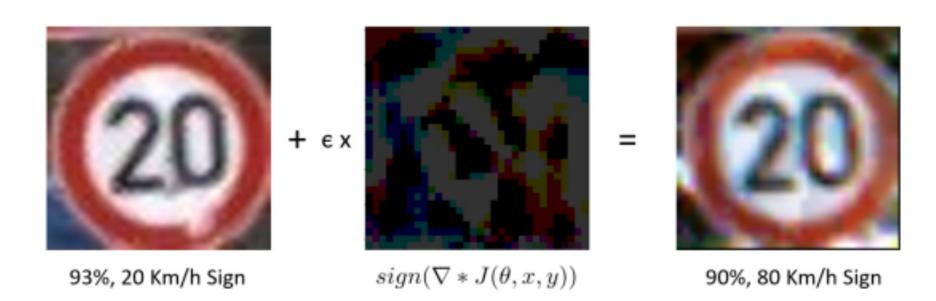
Tune your parameters!!

- Always tune parameters when comparing different settings / algorithms
- Never tune your parameters on the test set



ML is more than Curve Fitting

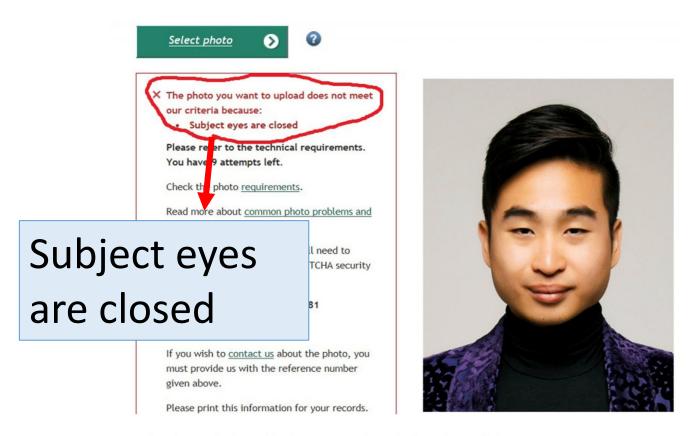
Real world is adversarial





ML is more than Curve Fitting

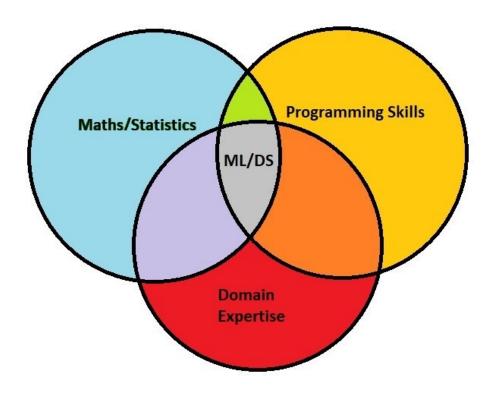
Build system works well for everyone



A screenshot of New Zealand man Richard Lee's passport photo rejection notice, supplied to Reuters December 7, 2016. Richard Lee/Handout via REUTERS

ML is more than Curve Fitting

Domain knowledge is important!



Thank you

Please log in MyUCLA for course survey

